Is the dispersion anomaly of the electron spectrum induced by the charge-density-wave in high-T_c superconductors?

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We propose that the presence of a rotationally symmetric charge density wave (CDW) with the modulation of 4-lattice constant in high-T_c superconductors is essentially responsible for an anomalous quasiparticle dispersion revealed recently by angle-resolved photoemission spectroscopy (ARPES) experiments. We elaborate clearly that the nodal quasiparticle is well-defined at low energies, while the dispersion breaks up at the energy E_1 and reappears at the energy E_2. Our results are in good agreement with both the ARPES and scanning tunneling microscopy experiments.

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Recently, scanning tunneling microscopy (STM) experiments have been performed to search for hidden electronic orders in high-T_c superconductors. A checkerboard pattern with the spatial four-unit-cell modulation for the local density of states was first seen around magnetic vortex cores in slightly overdoped samples by Hoffman *et al*. [1]. This kind of modulation pattern was also reported in later STM experiments, in zero field and in both the superconducting (SC) and normal states [2, 3]. In addition, the Fourier transform of the STM spectra (FT-STM) reveals four non-dispersive peaks at about $(\pm 2\pi/4, 0)$ and $(0, \pm 2\pi/4)$ in the normal [2] and SC state [3]. All of these experimental results indicate that a kind of charge density wave (CDW) order with a characteristic wave vector in the CuO bond direction of $q = 2\pi/4$ exists likely in high-T_c superconductors [4].

On the other hand, an intriguing anomalous quasiparticle dispersion was very recently observed in angle-resolved photoemission spectroscopy (ARPES) experiments [5, 6], i.e., a well-defined nodal quasiparticle dispersion is broken down between the two higher energies E_1 and E_2, which drops in a waterfall-fashion with a very low spectral weight. Below E_2, the quasiparticle dispersion reappears and disperses towards the zero center. These anomalous features were observed in several families of cuprates, in under-, optimal- as well as overdoped samples, and below or above the SC transition temperature. In hole-doped samples, the energies E_1 and E_2 are around 0.35 and 0.8 eV, respectively. While in the electron-doped samples ($Pr_{1-x}LaCe_xCuO_4$), the corresponding energies are found to be significantly larger with E_1 being around 0.6 eV [6]. The mechanism of these features is still unclear while it should be independent of the SC order. In addition, similar anomalous higher-energy features were also observed in the insulating cuprate $Ca_2CuO_2Cl_2$ [7]. Thus the mode coupling picture [8] can hardly account for these higher-energy behaviors because it is expected to happen only in metallic systems. Note that, it was proposed before that the CDW order may cause several other puzzling features seen in ARPES experiments [9, 10, 11]. Moreover, a connection between the ARPES and the FT-STM spectra was recently established [12, 13] through the autocorrelation of the ARPES (AC-ARPES) spectra. Therefore, it is natural and significant to ask whether the abovementioned anomalous dispersion observed in ARPES experiments can also be originated from the CDW order, which has already been detected by the STM experiments. We here answer this question clearly by studying the spectral function and the FT-STM based on a simple phenomenological model including the CDW order, though we note that a recent theory based on a new representation of the $t-J$ model with two-band fermions was also proposed for the anomaly [14].

At present, however, our knowledge on the origin and effects of the CDW order is still far from complete. What the phase diagram of such an order is and whether it exists in all cuprate materials are still unclear [9]. In fact, the STM experiments are mostly carried out on the $Bi_2Sr_2CaCu_2O_{8+x}$ and $Ca_{2-x}Na_xCuO_2Cl_2$ samples. While a similar four-unit-cell structure was also found in the $YBa_2Cu_3O_y$ samples by diffuse x-ray scattering measurements [15]. On the other hand, it seems widely believed that the CDW order may have the same physics as the stripe order [9], which has been seen in the $La_{2-x}Sr_xCuO_4$ sample [16]. In addition, the stripe order is suggested to exist in various doping region and to be the ground state of the cuprates [17]. Considering the above experimental and theoretical results, in this paper, we employ a phenomenological scenario that admits the existence of the CDW order to look into and elaborate its effect on the spectral function. The FT-STM spectra are also evaluated within our simple model and are compared with the STM experiments. We demonstrate that the CDW scattering is able to naturally lead to the

higher-energy anomaly in ARPES experiments and the non-dispersive peaks in the FT-STM spectra. Considering the robustness of this higher-energy anomaly, our results suggest that the CDW order be likely more robust in high-T_c superconductors.

We start with the following phenomenological Hamiltonian with a CDW order being taken into account,

$$H = H_{BCS} + H_{CDW}, \tag{1}$$

where H_{BCS} is the BCS-type Hamiltonian given by

$$H_{BCS} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} (\Delta_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} + h.c.), \tag{2}$$

with $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$, $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x - \cos k_y)/2$, and H_{CDW} is the CDW scattering term,

$$H_{CDW} = \sum_{\mathbf{Q}\mathbf{k}\sigma} (V c^{\dagger}_{\mathbf{k}+\mathbf{Q}\sigma} c_{\mathbf{k}\sigma} + h.c.), \tag{3}$$

with $\mathbf{Q} = (0, 2\pi/4)$ and $(2\pi/4, 0)$ being the CDW scattering wave vectors. Hereafter, the related parameters are chosen as $t = 0.35$ eV, $t' = -0.25t$. The chemical potential μ is determined by the doping density $\delta = 0.12$. We here use the isotopic s-symmetry CDW with the intensity $V = 0.1$ eV [18]. We have examined that our results are not sensitive to the slight changes of the chosen parameters and the robustness of our main conclusion with respect to the CDW scattering intensity V.

The electronic spectral function is given by $A(\mathbf{k}, \omega) = -1/\pi \mathrm{Im} G(\mathbf{k}, \omega + i\Gamma)$, where the retarded Green's function $G(\mathbf{k}, \omega + i\Gamma)$ is obtained by diagonalizing the Hamiltonian [Eq.(1)]. The intensity plots of $A(\mathbf{k}, \omega)$ are presented in Figs.1(a-d). We also plot the bare quasiparticle dispersions $\varepsilon_{\mathbf{k}}$ in the absence of the CDW scattering (the solid white lines) as a function of the momentum $\mathbf{k}$ for comparison. As seen, at low energies, the quasiparticle dispersions coincide almost with the bare ones. While they deviate from the bare ones when the momentum is close to $\mathbf{K_0} = (\pi/4, \pi/4)$. Then they break up at the energy E_1 around the momentum $\mathbf{K_0}$ and the quasiparticles would be ill-defined within $E_1 < E < E_2$. At the energy E_2 the dispersions reappear and disperse towards the $(0, 0)$ point. These results are independent on the SC order. While the energy E_i's for the electron-doped cuprates are larger than the corresponding ones for the hole-doped samples, namely, $E_1 \approx 0.35$ eV, $E_2 \approx 0.75$ eV in the hole-doped ones while $E_1 \approx 0.6$ eV, $E_2 \approx 0.95$ eV in the electron-doped ones. These results are well consistent with the experiments [5, 6]. E_i as a function of the CDW scattering intensity V is plotted in Figs.1(e) and (f). E_0 is the bare quasiparticle energy at the momentum $\mathbf{K_0}$. E_1 and E_2 approach to E_0 as V approaches to zero. As V increases, E_1 decreases and E_2 increases linearly. The main results are stable and robust as V changes slightly.

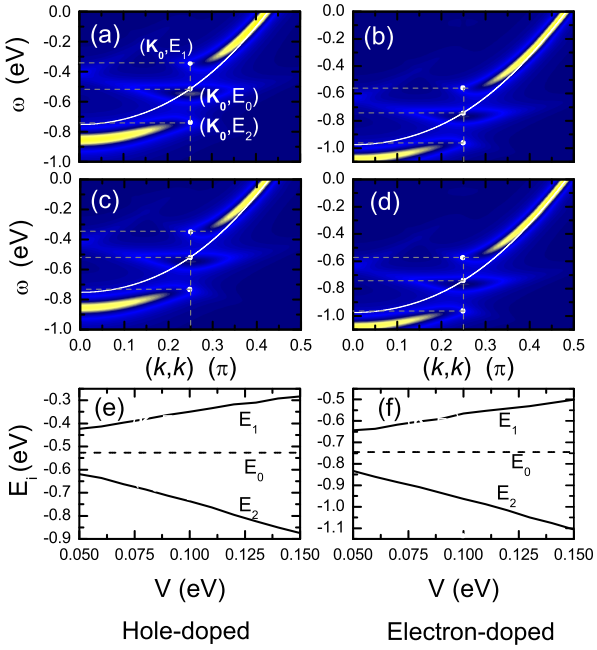

FIG. 1: (Color online) Panels (a-d) are the intensity plots of the spectral function as functions of the momentum and energy in the normal state (a,b) and SC state (c,d), respectively. The solid white lines represent the bare dispersions $\varepsilon_{\mathbf{k}}$. Panels (e,f) are the energies E_i versus the CDW scattering intensity V in the normal state (see the text). The left and right panels are for the hole- and electron-doped cases, respectively.

A sound explanation for the described anomalous higher-energy features can be given based on the following scattering characteristic illustration. The first Brillouin zone as well as the normal state Fermi surfaces of the electron- and hole-doped cuprates are presented in Fig.2(a). As seen, the Brillouin zone may be divided into sixteen parts in the presence of the CDW term, labeled as $'1'$ to $'16'$. When the CDW term acts on an electron in part $'i'$, it makes the electron hop to the four neighboring parts [19]. Let us assume that an electron at A_0 in region $'1'$ has the momentum (k, k) (i.e., along the diagonal direction). The effect of the CDW term makes it hop to A_{1-4} in the neighboring regions $'8, 4, 2, 11'$, respectively, as shown in Fig.2(a). The corresponding momentums for the electrons at A_{1-4} are $(k-\pi/2, k), (k, k+\pi/2), (k+\pi/2, k), (k, k-\pi/2)$, respectively. We present the bare dispersions for A_i $(i = 0-4)$ in Fig.2(b). The dispersions for the electrons at A_1 and A_4 (or A_2 and A_3) coincide because they are symmetric points. We can see from Fig.2(b) that the quasiparticle energy at A_0 is different from that at A_i as the momentum is far from $\mathbf{K_0}$. Thus the hopping from A_0 to A_i is difficult to occur because the energy conservation condition is not satisfied. As a result, the CDW term has little effect on the hopping for this case, namely, the quasiparticle is well-defined and the dispersion coincides almost with the bare one, as shown in Fig.1(a). When the momentum decreases and moves close to $\mathbf{K_0}$, the energy at

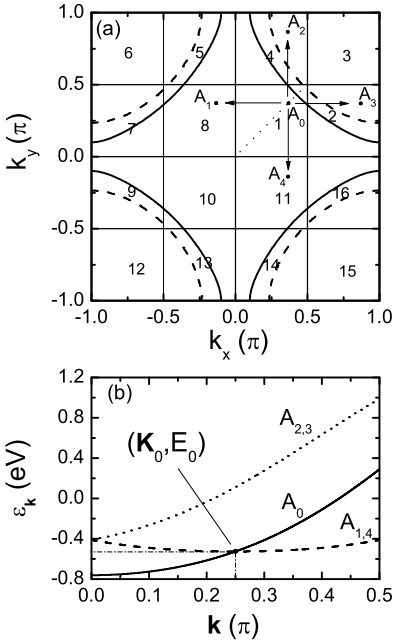

FIG. 2: (a) The normal state fermi surfaces for the hole-doped (solid line) and electron-doped (dashed line) cuprates, respectively. The scattering from $A_0 \to A_i$ indicates the hopping caused by the CDW term. (b) The bare dispersion of quasiparticles at A_0 (along the diagonal direction) and the corresponding dispersions of that at A_i for the hole-doped case.

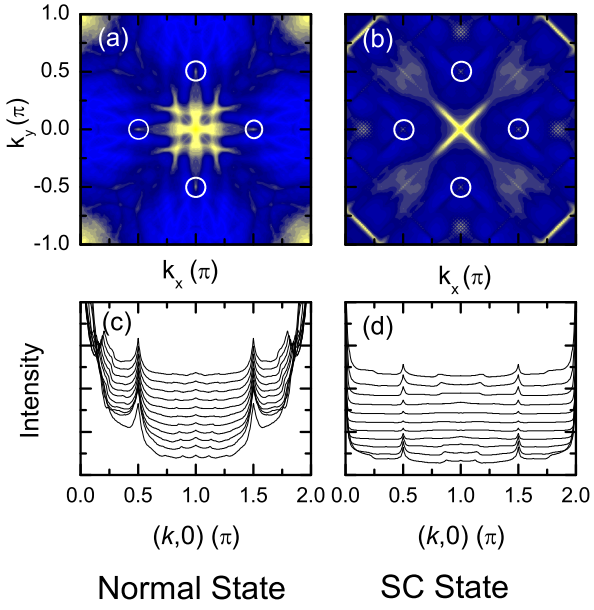

FIG. 3: (Color online) Panels (a) and (b) are the intensity plots of the AC-ARPES spectra $C(\mathbf{q},\omega)$ at the zero energy in the normal and SC state ($\Delta_0 = 0.04$ eV), respectively. White circles are used to denote the energy-independent peaks. Panels (c) and (d) are the two-dimensional cuts for the spectra along $(0,0)$ to $(2\pi,0)$ with the energy increasing from -0.02 eV to 0.02 eV (from the bottom to the top) in the normal and SC state, respectively.

A_0 is closer to that at A_1 and A_4. The CDW term influences significantly the dispersion. Thus it deviates from the bare one and the spectral weight reduces gradually. When the momentum reaches $\mathbf{K_0}$, the bare quasiparticle energy at A_0 just equals to that at A_1 and A_4, as seen in Fig.2(b), so that the hopping from A_0 to $A_{1,4}$ can occur easily, which destroys the state of the quasiparticle at A_0 and leads the dispersion to break up at this momentum. As a result, the dispersion is pinned by the CDW term and the quasiparticle is ill-defined. While, the quasiparticle dispersion is no longer pinned by the CDW term when the bounding energy is high enough (larger than E_2), and thus it reappears and disperses towards $(0,0)$ point. In fact, when the electron leaves the $\mathbf{K_0}$ point, the energy at A_0 is different from that at A_i and thus the quasiparticle is well-defined again.

In the SC state, the quasiparticle energy at A_0 is the same as that in the normal state along the diagonal direction, while that at A_i is changed due to the presence of the SC gap. Meanwhile, the quasiparticle energy at A_0 equals to that at $A_{1,4}$ at the momentum $\mathbf{K_0}$ because $A_{1,4}$ is along the nodal direction at this momentum. Thus the addressed anomaly depends weakly on the SC order parameter Δ_0. For the electron-doped cases, since the Fermi momentum $\mathbf{K_F}$ along the diagonal direction is greater than that of the holed-doped sample, as seen from the Fermi surfaces shown in Fig.2(a), the bounding energy at $\mathbf{K_0}$ is larger. As a result, the anomalous energies E_1 and E_2 are larger than those of the hole-doped ones, consistent with the experimental results [6].

We now turn to address the FT-STM spectra in hole-doped cuprates. As we mentioned above, the FT-STM spectra can be related to the ARPES spectra through the AC-ARPES function $C(\mathbf{q},\omega)$, given by [12],

$$C(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{k}} A(\mathbf{k},\omega)A(\mathbf{k}+\mathbf{q},\omega). \qquad (4)$$

Very recently, it was concluded experimentally that the FT-STM spectra are in good agreement with the AC-ARPES spectra at low energies for various doping densities [13]. Therefore, we here use the AC-ARPES to deduce the FT-STM spectra and compare the results with the STM experiments. The calculated intensities of the AC-ARPES spectra at zero energy, in the normal and SC state, are shown in Fig.3(a) and Fig.3(b), respectively. The log scale is used so that the weak features can be revealed. As shown, four peaks appear at the momentums $(\pm 2\pi/4, 0)$ and $(0, \pm 2\pi/4)$. These peaks are independent of the energies, as seen more clearly in Figs.3(c) and (d), which are the two-dimensional cuts of the spectra for the energies from -0.02 to 0.02 eV. These non-dispersive peaks in the FT-STM spectra were observed experimentally in the normal state [2]. In the SC state, while they are suppressed by the SC order, they were also indeed observed by STM experiments as well [3].

The consistency between the FT-STM and AC-ARPES

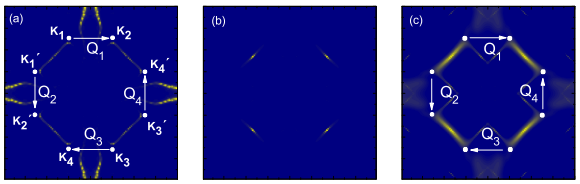

FIG. 4: (Color online) Panels (a) and (b) are the intensity plots of ARPES spectra at zero energy in the normal and SC state, respectively. Panel (c) is the replotting of the spectra in the SC state while the log scale is used.

spectra indicates that the non-dispersive peaks may be explained based on the quasiparticle interference model [20, 21], i.e., the momentums of the peaks in FT-STM spectra are just the wave vectors that connect the tips of the constant energy contour. Based on this picture, the various dispersive peaks observed by STM experiments in the SC state [20, 22] are reproduced successfully. At present, in the presence of the CDW order, the intensity plots of the ARPES spectra at zero energy are depicted in Figs.4(a) and (b)/(c) for the normal state and SC state, respectively; since the ARPES spectrum is reduced to a dot along the nodal direction in the SC state [Fig.4(b)], we re-plot it by using a log scale in Fig.4(c) to reveal the weak features caused by the CDW order. As we discussed above, the ARPES spectra break up at the momentums $\mathbf{K_i} = (\pm\pi/4, q)$ and $\mathbf{K'_i} = (q, \pm\pi/4)$ because of the CDW scattering, leading to the tips of the spectra at these momentums. In the corresponding AC-ARPES spectra, the peaks appear at the momentums $\mathbf{Q_i}$ that connect the tips of the ARPES spectra, as denoted in Figs.4(a) and (c). As a result, although the CDW order has a very weak effect on the low energy ARPES spectra, which is difficult to be detected directly by the ARPES experiments, the non-dispersive peaks induced by the CDW order appear clearly in the AC-ARPES spectra (or the FT-STM spectra) and can be detected firmly by the STM experiments.

To conclude, based on a phenomenological model, we have for the first time elaborated that the CDW scattering is able to cause the intriguing dispersion anomaly observed in the ARPES spectra for both hole-doped and electron-doped samples as well as the non-dispersive peaks in the FT-STM spectra. A clear physical picture of the mechanism was presented based on the scattering analysis in the presence of the CDW order.

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